Ionization energy of nanostructures using the reciprocal randi´c index

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Abstract

Topological indices are constant of graph, used to study quantitative structure activity relationship (QSAR) and quantitative structure Properties relationship (QSPR). In addition to mathematics, graph theory is used in physics, chemistry, pharmacology, genetics, and also some other sciences. These indices are widely used to illustrate the relationship between molecular structure and physical and chemical properties. This study aims to obtain a simple model based on graph theory to predict the Ionization Energy of phenacenes with chemical formula $C_{4n+2}H_{2n+4}$. Therefore, we first calculated the Reciprocal Randi´c Index for the family. Reciprocal Randi´c index, RR (G) is defined by RR (G)=$\sum_{ij\in E}\sqrt{didj}$ The Ionization Energy of phenacenes was calculated using Gaussian 09 software and the experimental data of references were compared with those mentioned in valid papers. The prediction of Ionization Energy about a very high accuracy through reciprocal Randi´c index, with R^2=0.9873. The prediction is given by: $E_{Ionization} = 0.0002(RR)^2 - 0.0425(RR) + 8.787$.

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